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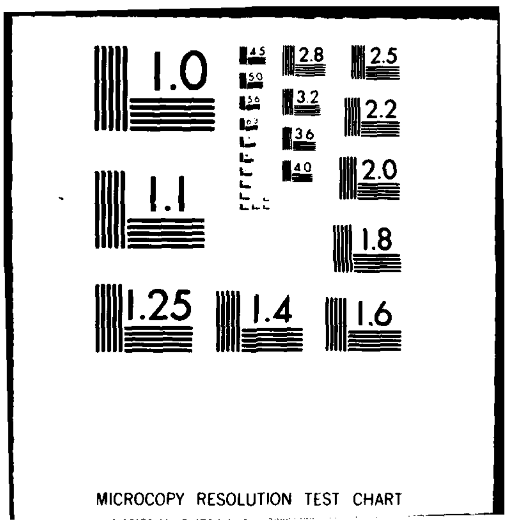
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ANNUAL REPORT

SURFACE EFFECTS ON PLASTIC DEFORMATION

BY

R.J. Arsenault

and

I.R. Kramer

TO

OFFICE OF NAVAL RESEARCH

CONTRACT NUMBER

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UNIVERSITY OF MARYLAND
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The present computer simulation study of the dislocation distribution near the surface is based upon a modified one-dimensional dislocation model which considers the line tension of a dislocation loop, and the image forces. If the dislocations are generated from a surface source and move by thermal activation over randomly distributed short range barriers, an inverse pile-up is created. A dislocation density gradient exists up to a depth of

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~60 μm, for a total of twenty dislocations generated. During unloading, the last few dislocations generated leave the crystal rapidly, and within three hours to two weeks the dislocation density gradient essentially disappears (depending upon the parameters used). This is in agreement with the experimental results.

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INTRODUCTION

Whether plastic deformation induces a soft surface or a hard surface has been a controversy for the past fifteen years or more. The experimental evidence of a higher dislocation density at surface or in the core region following plastic deformation seems often contradictory. There has been several mechanisms proposed which would lead to a lower dislocation density in the near surface region of a metal with a clean surface. The object of the present study is to develop a model which will result in a higher dislocation density in the near surface region.

The present model is based on two well-known facts: (1) Surface sources can be activated at a lower stress than sources in the interior of a sample. (2) Thermally activated dislocation motion from a source will create an inverse pile-up. Therefore, if all dislocations are generated from a surface source and their motion is controlled by thermal activation, then there will always be a higher dislocation density in the near surface region during loading.

During the unloading stage, however, the dislocations will travel out of the crystal by a superposition of the following factors: (1) Line tension due to the curvature of dislocation loop (2) Attractive force by image dislocation arrays, which are mirror images to the real dislocations. (3) Repulsive forces by those dislocations of the same sign, lying ahead in the pile-up. Therefore, some extra barriers

may have to be introduced which will stop the dislocations from exiting too easily. The intersection of a secondary dislocation slip system with the primary ones will create these extra barriers.

DISCUSSION OF RESULTS

The present study of surface dislocation sources will be concentrated on the following three models: 1. A one-dimensional model with one slip system: A group of straight-edge dislocations parallel to each other are created from a surface source and move on a slip plane by an applied shear stress. In addition, line tension terms are included which take into account the circular nature of dislocation loops. Also, the image forces are considered. 2. A two dimensional model with two slip systems: Two systems of parallel-straight-edge dislocations lying on two slip planes intersecting at 70° which can operate simultaneously from each surface source. 3. A three dimensional model with two slip systems: The static interaction between various configurations of two systems of nonparallel, noncoplanar straight edge dislocations of slip system $[10\bar{1}]$ $(\bar{1}2\bar{1})$ and $[0\bar{1}\bar{1}]$ $(\bar{2}1\bar{1})$ are being considered.

Isotropic linear elasticity is always assumed in the present study. Only room temperature is considered.

Model 1

The thermally activated motion of straight dislocations from a source under an applied stress will create an inverse dislocation pile-up on a slip plane with randomly distributed short range barriers (SRB) (Fig. 1). The equilibrium position of a dislocation is determined by a static force balance. Normally, under an applied stress, a dislo-cation will be pushed against a (SRB) with a resultant positive effective stress such as to lower the activation energy required for jumping forward. However, there are occasions, although very few, that a dislocation "floats" in between two SRB's with zero effective stress and thus not in a position to jump any SRB yet.

In order to relax the present restriction of a straight dislocation, the backward force component of the line tension of a dislocation loop is considered. If the source is at the surface of the crystal, as in Fig. 2, a further term is needed, i.e., the algebraic sum of the image forces by an array of inverse pile-up image dislocations. The result of adding these two extra backward force terms adds to the difficulty of operating a dislocation source.

The actual distribution of dislocations as a function of time depends to a large extent on the chosen values of the parameters such as τ_o, the stress for dislocation motion at 0 K, τ_s, the source operating stress, ΔG_o, the activation energy at zero effective stress, and finally, ΔX_{AV}, the average spacing among randomly distributed SRB's. In the

present study, because the exact values for copper are not known, some reasonable estimates are made in choosing the appropriate values of τ_p, τ_s and ΔX_{AV}. The applied stress, τ_a, is chosen so as to give a reasonable generation time for twenty dislocations. A range of estimated ΔG_o values were examined.

It is found that, in spite of the differences in ΔG_o, the penetration depth of the first dislocation generated in an array of twenty is always between 500 and 600 μm. This indicates that the dislocation distribution is approximately constant for a given number of generated dislocations. If the dislocation density distribution is considered, (Fig. 3) the density changes rapidly at about 100 μm. For depths greater than 100 μm the density is much less than for a depth up to 100 μm. (This is in agreement with the experimental results of Kramer who has stated that the hard layer extends into a depth of approximately 100 μm.)

As soon as the three dislocations nearest to the surface leave the crystal during recovery, the dislocation density established by the inverse pile-up in front of the source essentially disappears. After three more dislocations leave the crystal, a reversed dislocation density gradient is developed, i.e. a lower density exists near the surface. The time necessary for this reversed gradient to demonstrate itself will be termed "recovery time". The dislocation distributions after recovery are similar for the small range of ΔG_o values compared here. (The values of ΔG_o choosen represent

estimates of ΔG_o for copper).

As can be seen from the effects of different ΔG_o in Table 1, both the generation and the recovery times are very sensitive to a change in ΔG_o. Therefore, a very accurate experimental determination of ΔG_o for copper is needed.

The present study, therefore, points out the possibility of a new interpretation of the controversy between "hard surface" and "hard core" theories in plastic deformation. The initiation of plastic deformation occurs at the surface and leads to higher dislocation density at the surface which means the existence of a hard surface, but if the sample is left for a long enough period for recovery to take place such that a reversed dislocation density gradient develops, then a hard core exists.

Model 2

The two dimensional model is based on the dynamic motion of parallel edge dislocations moving on two intersecting slip planes at an angle α, as in Fig. 4. For FCC metals, {111} slip planes intersect at $\alpha = 70°$. For each dislocation present, the interaction with all other dislocations and their images on both planes have to be considered (Fig. 5). The applied stress component on the secondary slip plane is determined from the Schmid factor which corresponds to a maximum probability of secondary slip. A number of static interaction for various dislocation configurations has been studied. The dislocations on the primary and the secondary systems seem to be moving in a cooperative mode. As the

leading dislocations approach the junction on their respective plane, they encounter increasingly large repulsive forces. Therefore, it seems that if both systems are to be operated simultaneously, they will block each other at the junction.

If the inverse pile-up already existed on the primary plane when the secondary system is activated, the result indicate that there are open-gate and close-gate configurations for the primary dislocations. In other words, the secondary dislocations can easily move through the junction if the primary dislocations are preferentially distributed; whereas in other cases, it will be extremely difficult to pass it.

Model 3

In FCC metals, edge dislocations on the secondary and primary slip planes are never parallel to each other. In order to represent the real orientation, a three dimensional model is needed (Fig. 6). The interaction force between the primary and the secondary dislocations is thus the general case of a non-parallel, non-coplanar dislocation pair. The correspondence of this three-dimensional model and the previous two-dimensional model can be understood by looking at the viewing plane perpendicular to the intersection line $\bar{M}N$, (Fig. 7) with the dislocation penetration spots P and S considered as the equivalent two-dimensional dislocation locations. Therefore, when the two dislocations are equidistant to the junction point O and are on the same side from O, they are actually intersecting each other along MN

somewhere. As the dislocations intersect each other, an attractive junction should have formed which would require approximately 10^2 eV to break them apart in either direction.

An interesting fact is that the total interaction force between a general dislocation pair is independent of the nearest distance between them. As the dislocations approach each other, the interaction region simply becomes more localized with higher force per unit dislocation length near the points of smallest distance. An attempt is made to simplify the model by considering only the length of dislocation with an interaction force per b greater than some threshold value. Since the total force is a constant, as the dislocations approach each other, the effective length become smaller and the effective interaction force per b will thus increase. It turns out that the effective length is a linear function of the nearest distance. The attractive force toward the junction on both planes seems to agree with the attractive junction formation arguments.

The plan is to incorporate these three dimensional results into the two dimensional program. For, from a computer time consideration it would be impossible to do dynamic simulations with a three dimensional model.

TABLE 1

ΔG_o (eV)	Generation time (sec)	Recovery time (sec)
0.75	1.96	2.8×10^3 (1.3 hr.)
0.85	27.3	3.0×10^5 (4 days)
1.05	1040	3.9×10^8 (10 years)

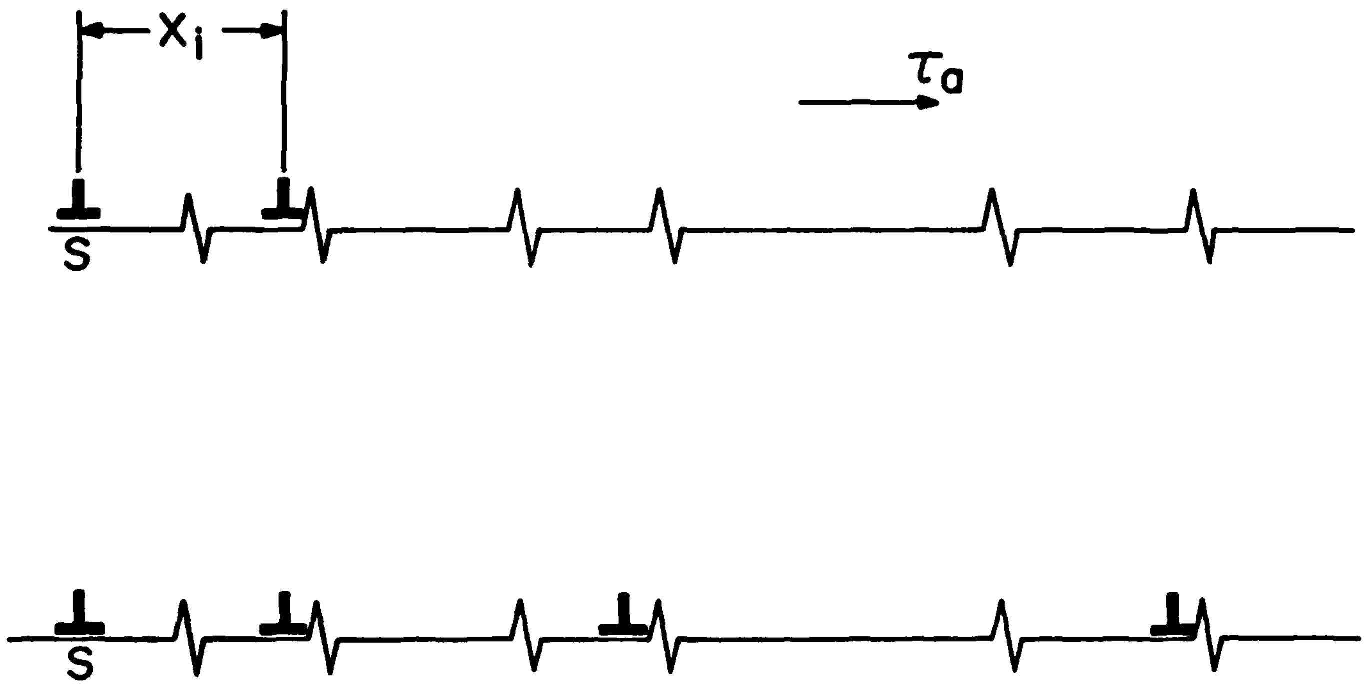


Fig. 1. Inverse pile-up of dislocations from an operating source.

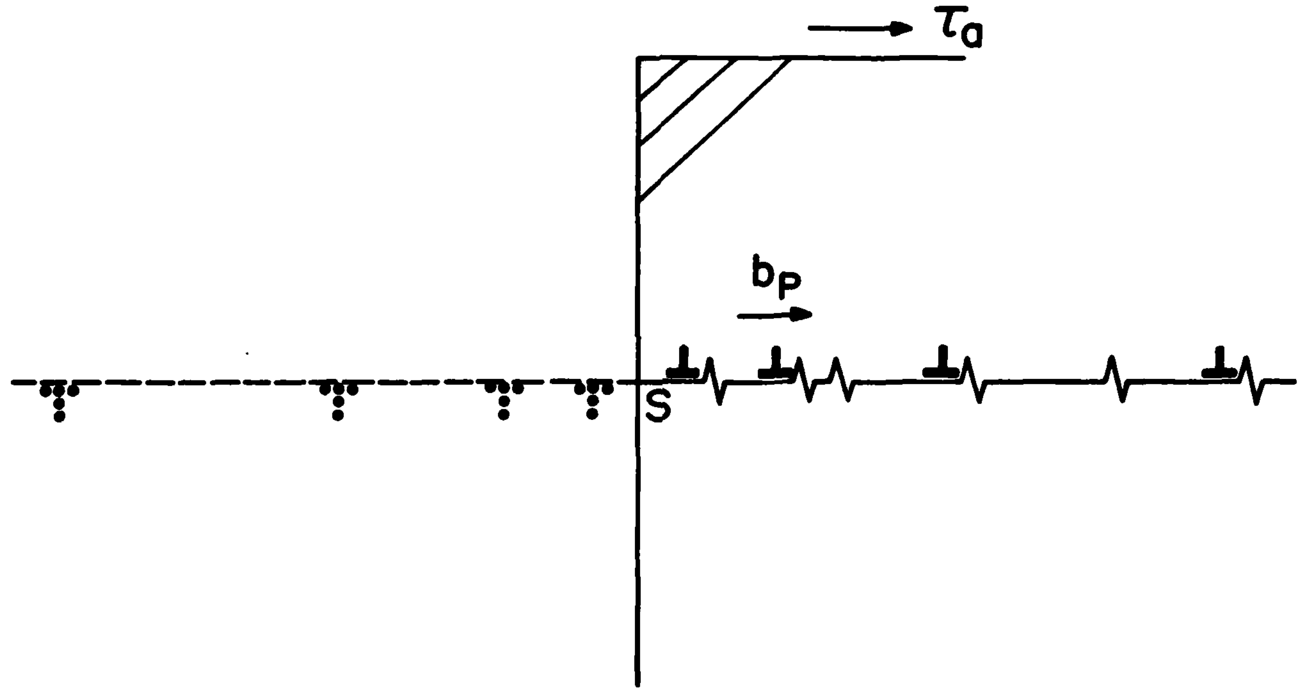


Fig. 2. A one-dimensional model of a surface source and image dislocations.

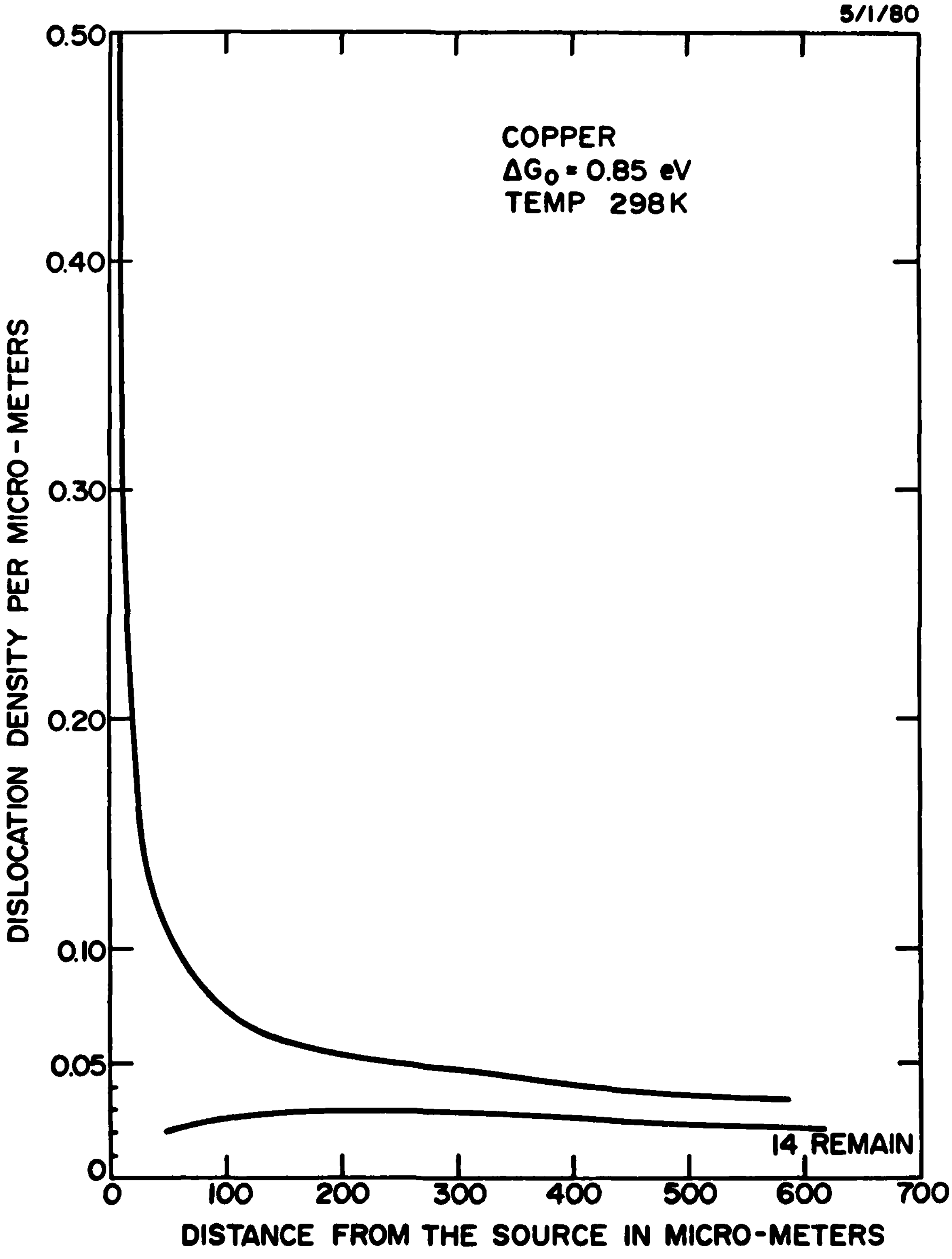


Fig. 3. Dislocation density as a function of depth beneath surface before and after recovery.

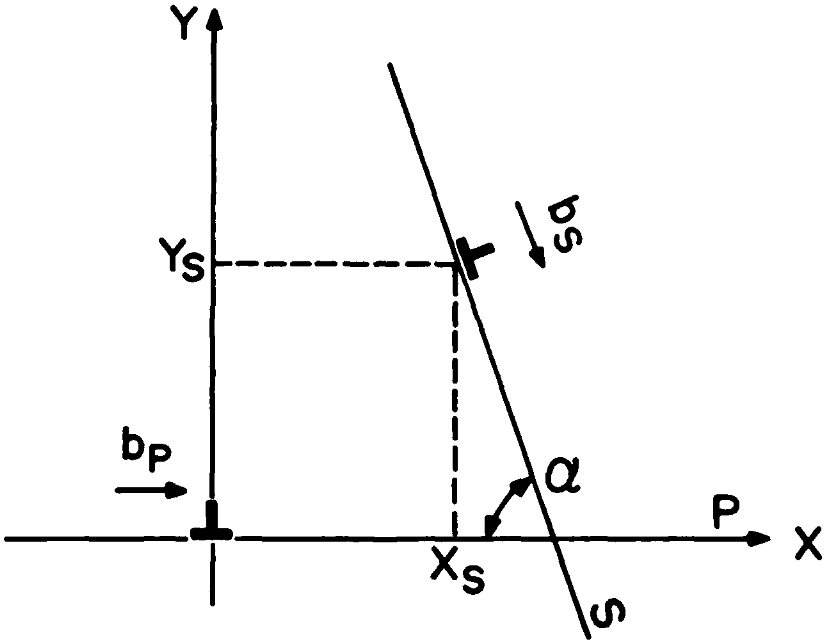


Fig. 4. Interaction between dislocations on the primary and secondary slip planes.

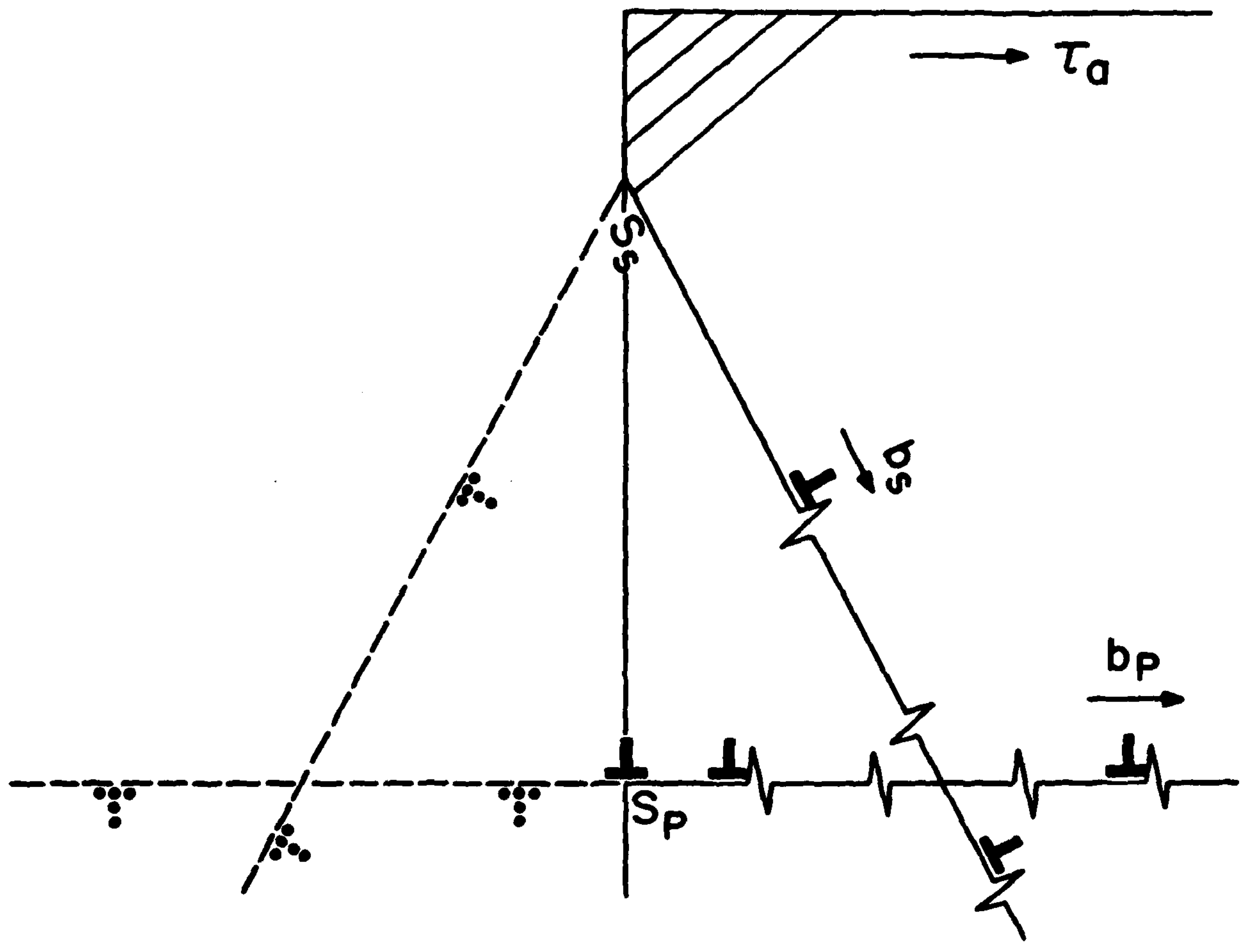


Fig. 5. A two-dimensional model with two slip systems and their image dislocations.

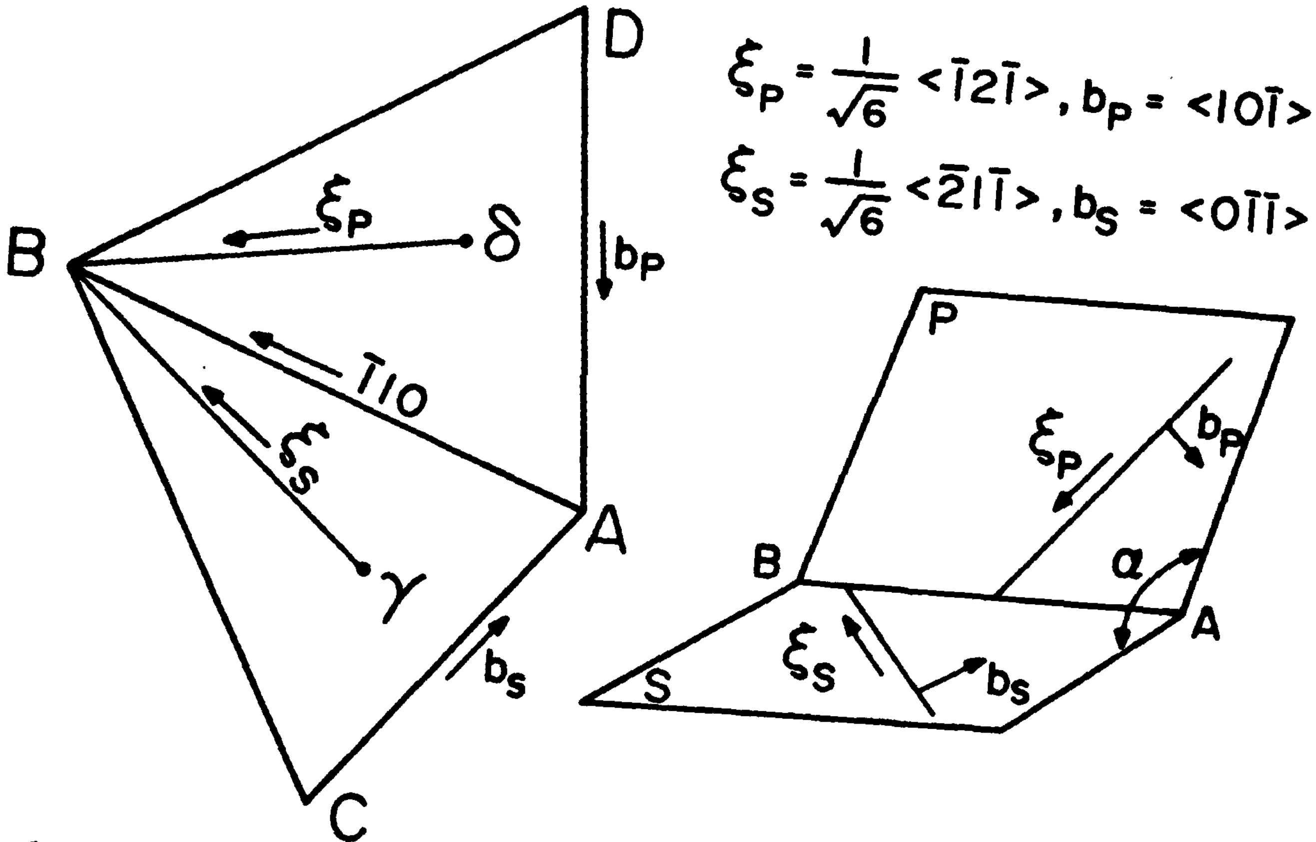
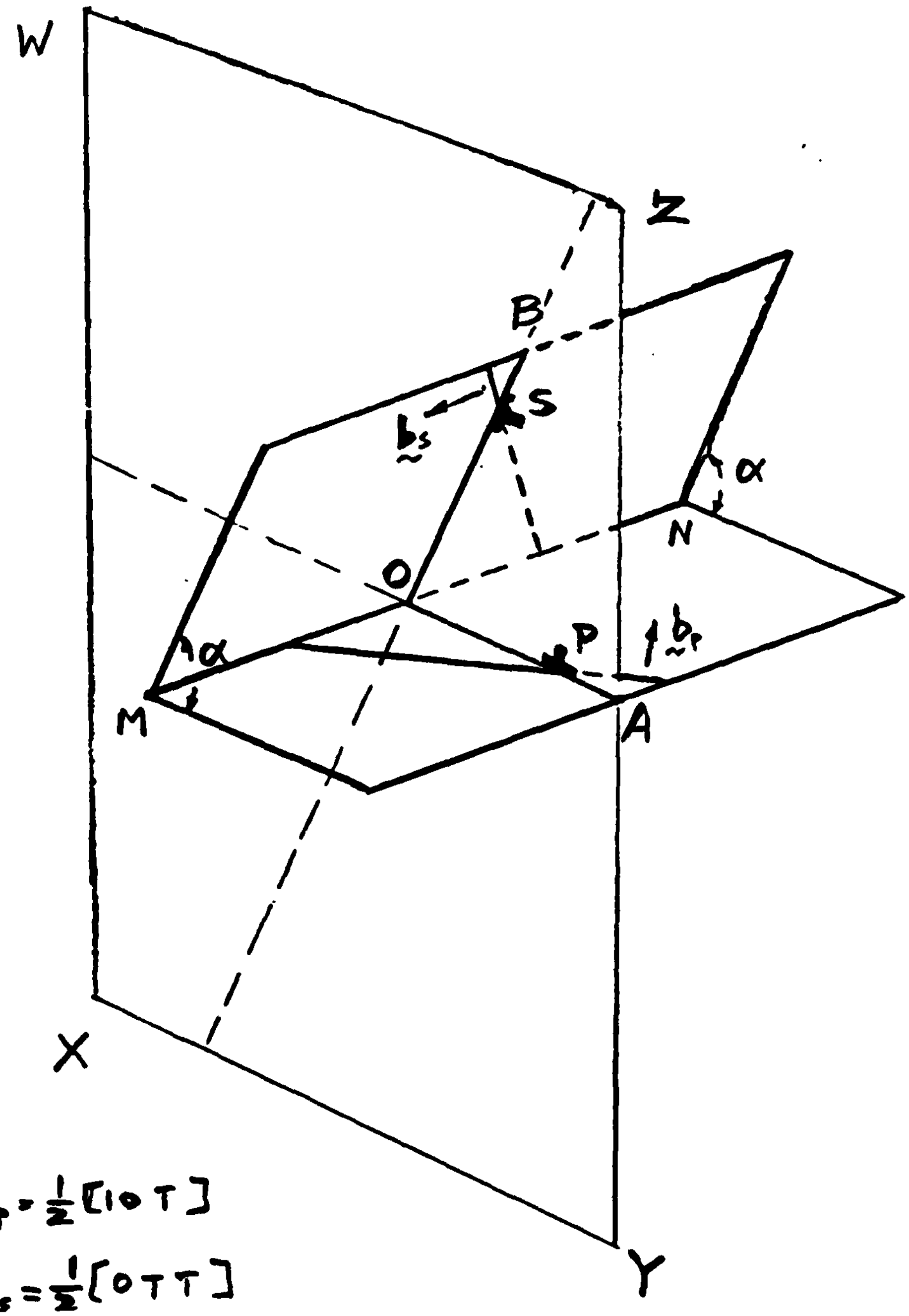


Fig. 6. A three-dimensional model of two slip systems.



$$\underset{\sim}{b}_p = \frac{1}{2}[10\bar{1}]$$

$$\underset{\sim}{b}_s = \frac{1}{2}[0\bar{1}\bar{1}]$$

Fig. 7. The correspondence between 2- and 3-dimensional models.